Supporting Information

Lysosome-Targeting Bis-terpyridine Ruthenium(II) Complexes: Photophysical Properties and *in vitro* Photodynamic Therapy

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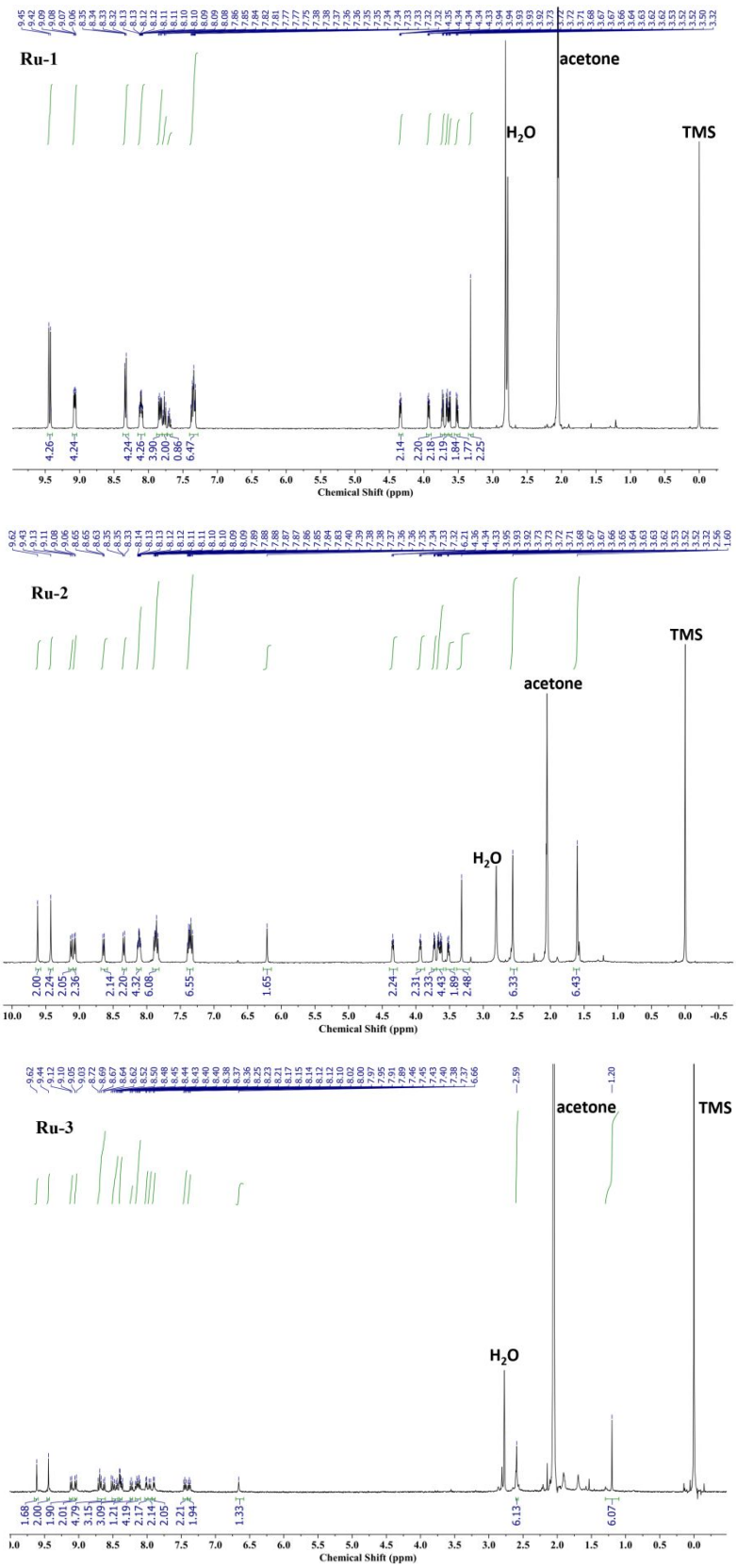


Figure S1. ^{1}H NMR (400 MHz, acetone-d_6) spectra of complexes **Ru1**-**Ru3**.

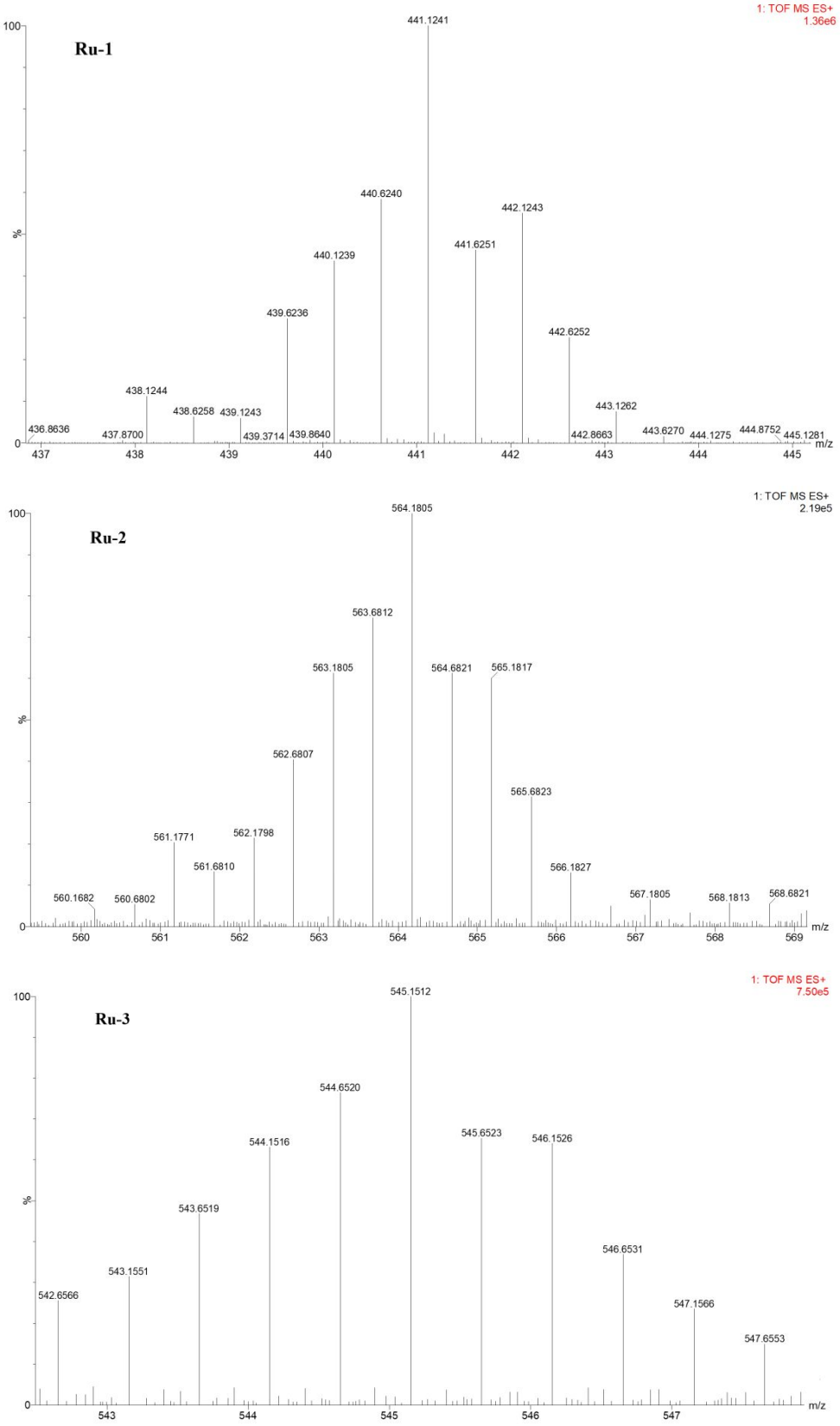


Figure S2. ESI-HRMS spectra of complexes **Ru1**-**Ru3**.

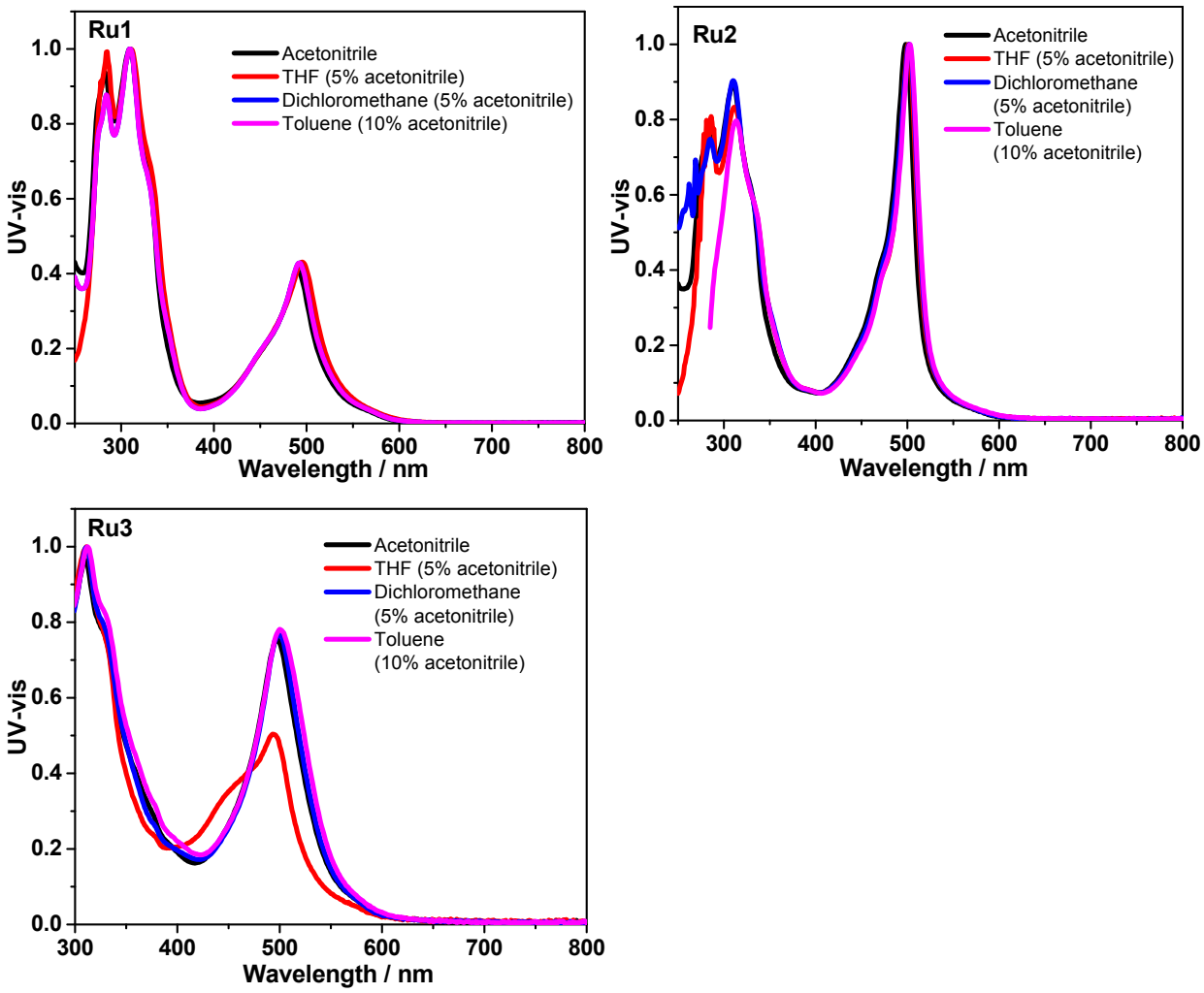


Figure S3. Normalized UV-vis absorption spectra of **Ru1-Ru3** in different solvents.

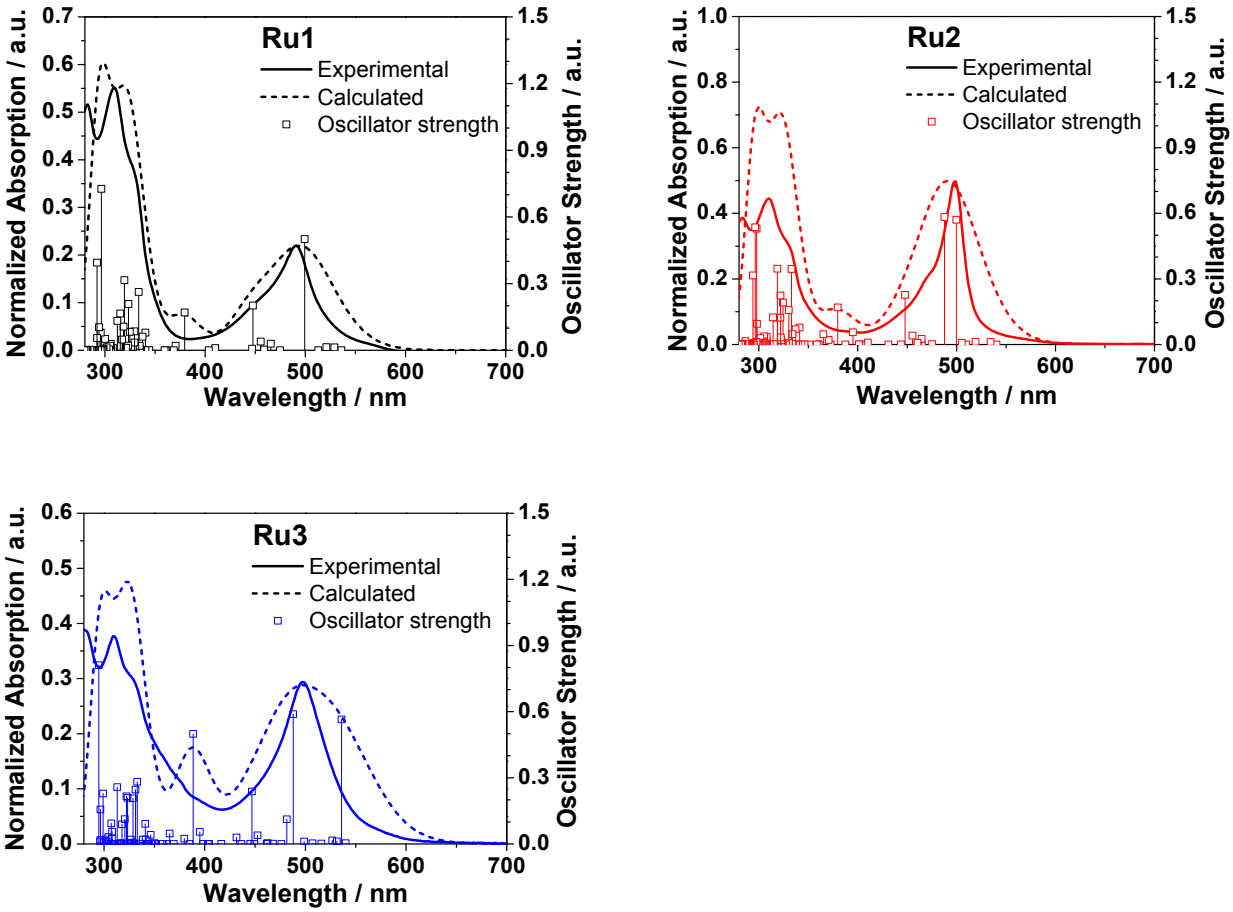
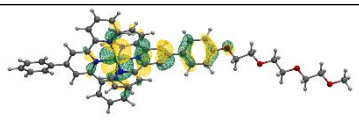
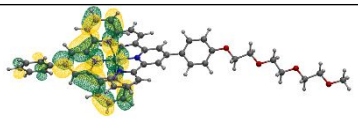
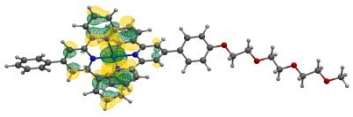
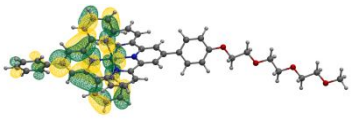
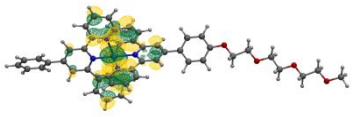
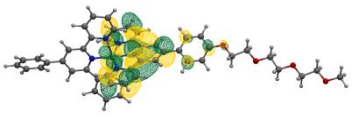
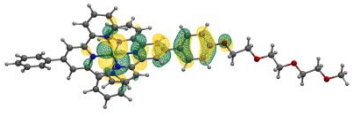
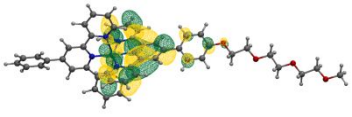
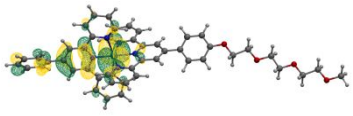
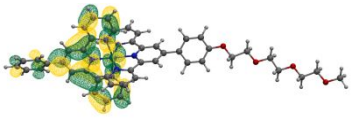
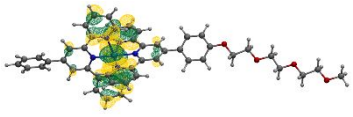
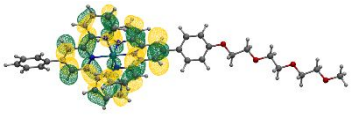
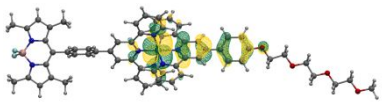
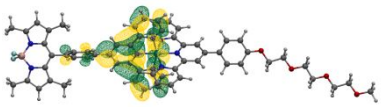
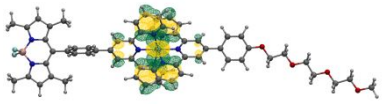
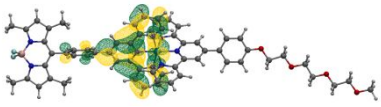
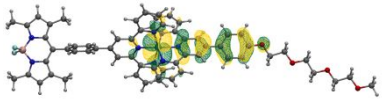
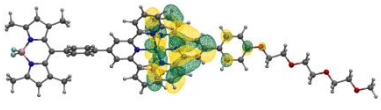


Figure S4. Comparison of the normalized experimental and calculated absorption spectra of **Ru1**–**Ru3** in acetonitrile. The calculated spectra used PBE1PBE functional with LANL2dz/6-31G* basis and were red shifted by 0.40 eV to match the respective experimental spectra.

Table S1. NTOs of the major transitions contributing to the absorption bands at 400-600 nm for Ru1-Ru3, calculated by TDDFT method with PBE1 functional and LANL2dz/6-31G* basis set in acetonitrile. The wavelengths in parenthesis are the values after 0.40-eV red shift.

Complex	Excited states and properties	Hole	Electron
Ru1	S_1 457 nm (536 nm) *f=0.000*		
	S_2 452 nm (529 nm) *f=0.013*		
	S_3 446 nm (521 nm) *f=0.014*		
	S_5 430 nm (499 nm) *f=0.500*	 60%	 60%
		 37%	 37%
	S_{10} 391 nm (447 nm) *f=0.202*		
Ru2	S_1 460 nm (540 nm) *f=0.000*		
	S_2 456 nm (534 nm) *f=0.012*		
	S_6 430 nm (499 nm) *f=0.571*	 56%	 56%

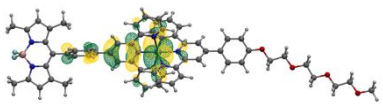
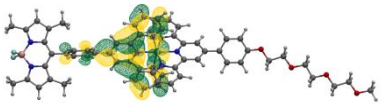
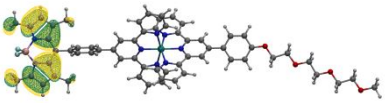
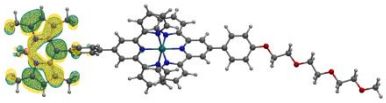
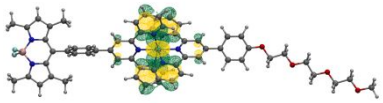
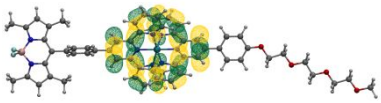
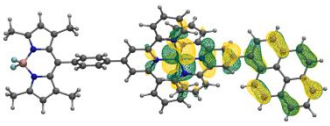
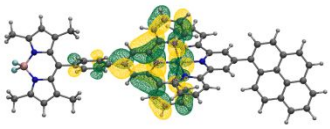
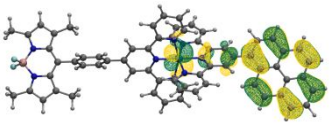
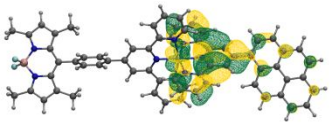
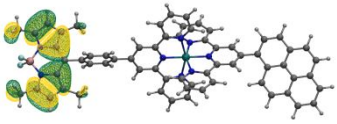
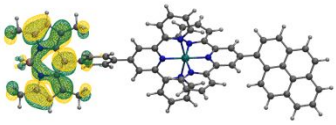
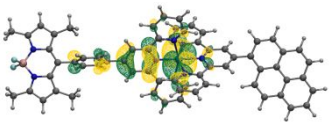
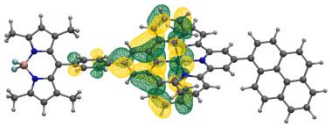
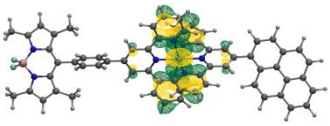
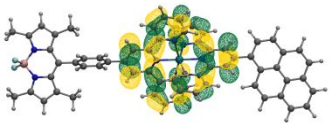
		 41%	 41%
	S_7 421 nm (487 nm) *f=0.583*		
	S_{14} 391 nm (447 nm) *f=0.227*		
Ru3	S_1 460 nm (540 nm) *f=0.003*		
	S_2 457 nm (536 nm) *f=0.565*		
	S_8 421 nm (487 nm) *f=0.589*		
	S_9 417 nm (481 nm) *f=0.112*		
	S_{17} 391 nm (448 nm) *f=0.238*		

Table S2. NTOs of the major transitions contributing to the absorption at 350-400 nm for Ru1-Ru3, calculated by TDDFT method with PBE1 functional and LANL2dz/6-31G* basis set in acetonitrile. The wavelengths in parenthesis are the values after 0.40-eV red shift.

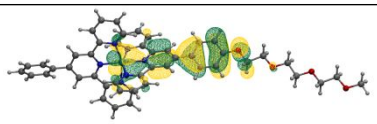
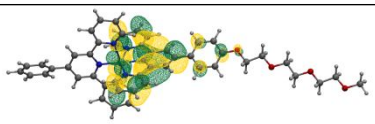
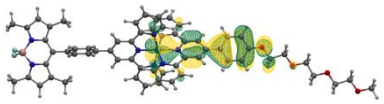
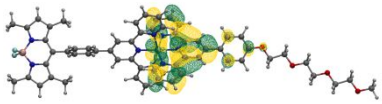
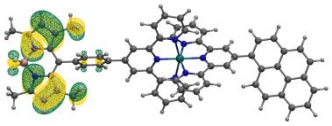
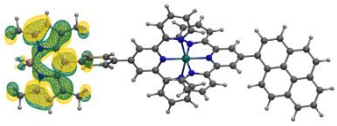
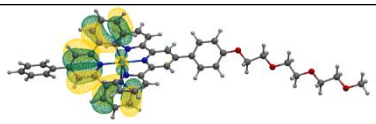
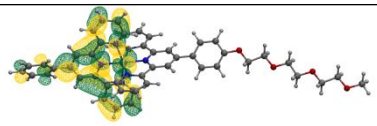
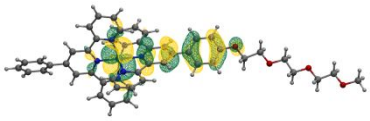
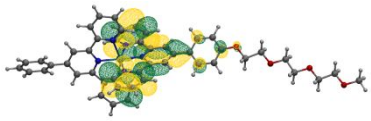
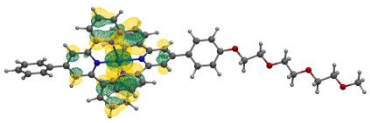
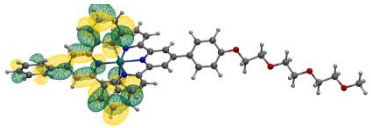
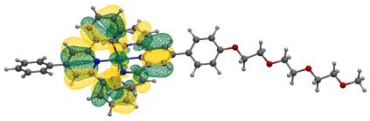
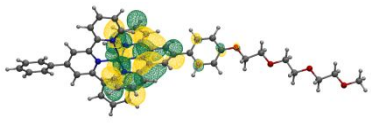
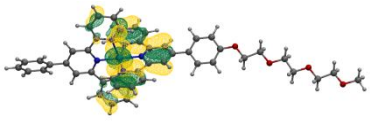
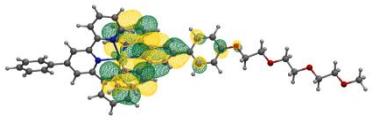
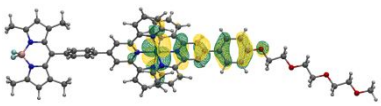
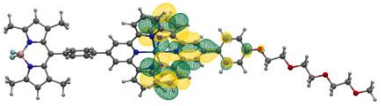
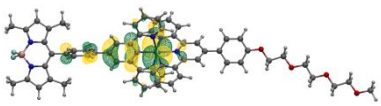
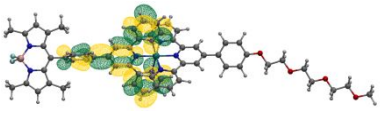
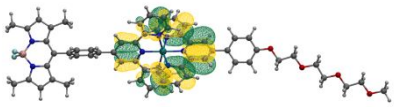
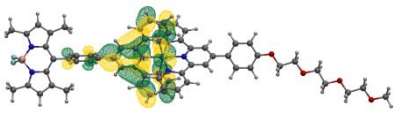
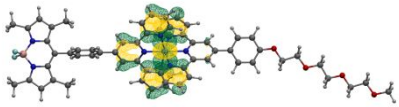
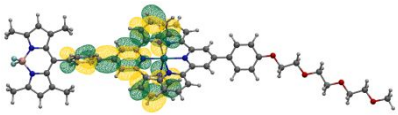
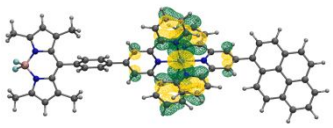
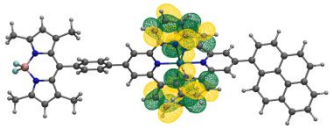
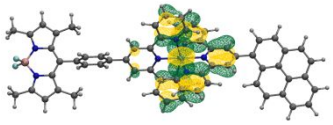
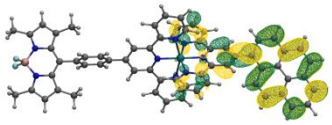
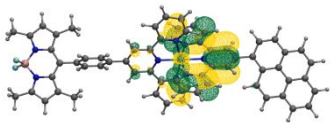
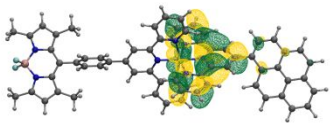
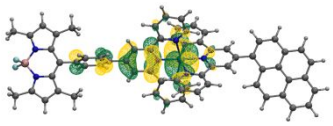
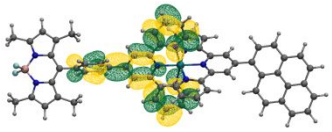
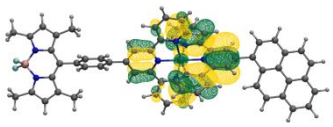
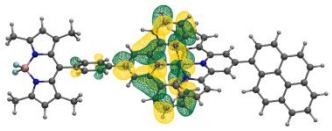
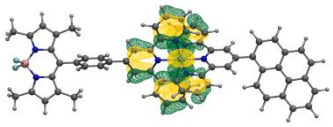
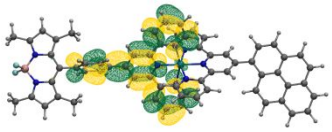
Complex	Excited states and properties	Hole	Electron
Ru1	S_{14} 338 nm (379 nm) *f=0.170*		
Ru2	S_{23} 338 nm (379 nm) *f=0.170*		
Ru3	S_{25} 350 nm (394 nm) *f=0.055*		

Table S3. NTOs of the major transitions contributing to the absorption at 280-350 nm for Ru1-Ru3, calculated by TDDFT method with PBE1 functional and LANL2dz/6-31G* basis set in acetonitrile. The wavelengths in parenthesis are the values after 0.40-eV red shift.

Complex	Excited states and properties	Hole	Electron
Ru1	S_{20} 307 nm (341 nm) *f=0.080*		
	S_{26} 301 nm (333 nm) *f=0.263*		
	S_{30} 293 nm (324 nm) *f=0.208*		
	S_{33} 290 nm (320 nm) *f=0.315*	 51%	 51%
		 44%	 44%
Ru2	S_{39} 301 nm (333 nm) *f=0.346*		
	S_{42} 298 nm (330 nm) *f=0.158*		
	S_{44} 294 nm (325 nm) *f=0.192*	 55%	 55%
		 37%	 37%

Ru3	S_{45} 301 nm (333 nm) *f=0.282*		
	S_{48} 299 nm (331 nm) *f=0.247*	 59%	 59%
		 36%	 36%
	S_{51} 297 nm (328 nm) *f=0.207*		
	S_{57} 293 nm (324 nm) *f=0.209*	 49%	 49%
		 42%	 42%

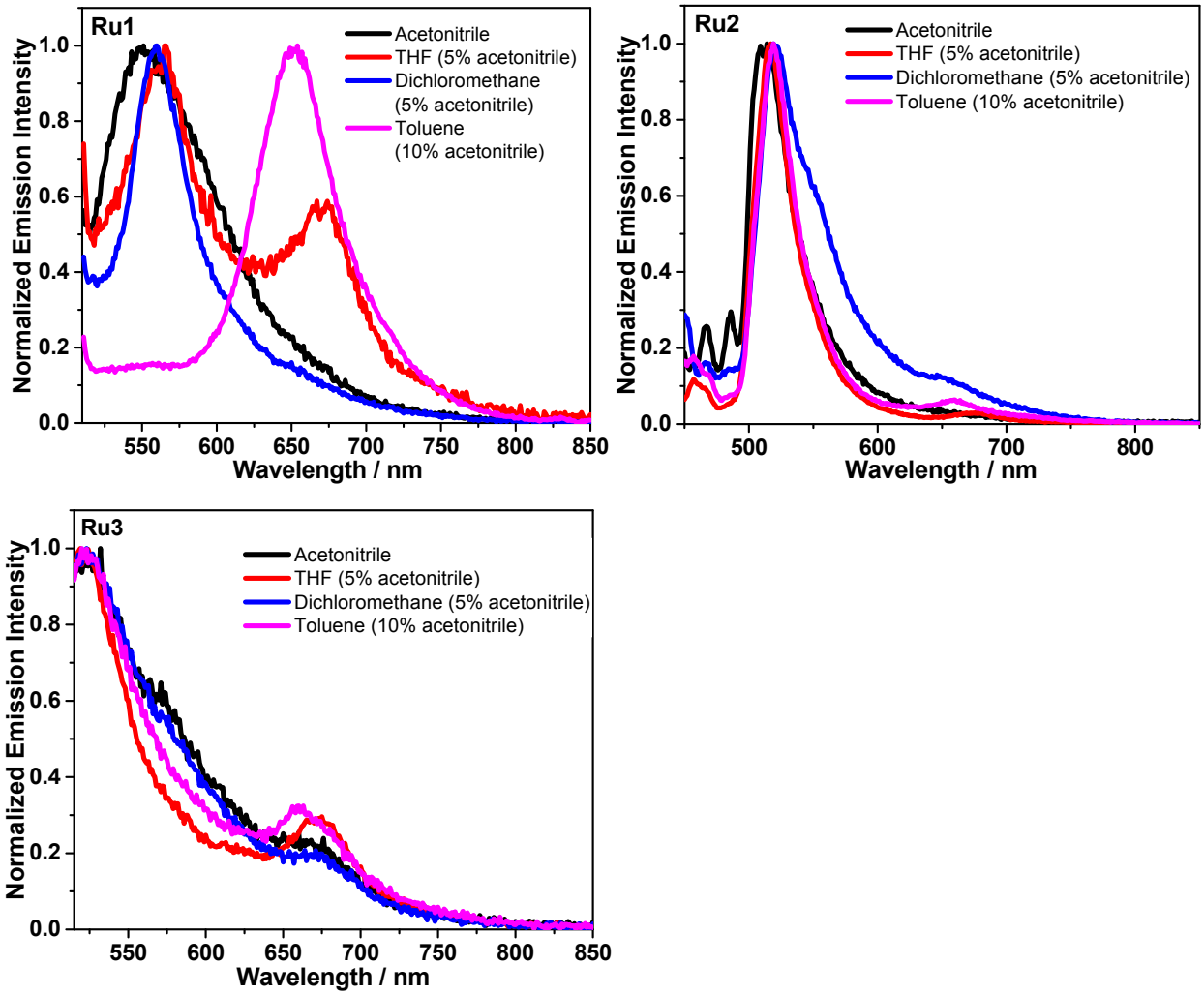


Figure S5. Normalized emission spectra of complexes **Ru1-Ru3** in different solvents (λ_{ex} = 436 nm).

Table S4. Emission characteristics of complexes **Ru1**-**Ru3** in different solvents at room temperature.[a]

	λ_{em}/nm; Φ_{em}			
	CH_3CN	THF (with 5% CH_3CN)	Dichloromethane (with 5% CH_3CN)	Toluene (with 10% CH_3CN)
Ru1	551; 0.0024	564, 674; 0.0040	559, 650; 0.0049	652; 0.074
Ru2	513; 0.0051	516, 673; 0.068	520, 646; 0.065	518, 658; 0.075
Ru3	525, 668; 0.0011	522, 674; 0.0012	522, 670; 0.0015	522, 659; 0.0013

[a] λ_{em} = 436 nm. The emission lifetimes were too short or the emission signals were too weak to allow for the lifetimes to be measured on our instrument.